Theory for superconductivity in (Tl,K)Fe_xSe_2 as a doped Mott insulator

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Abstract. - Possible superconductivity in recently discovered (Tl,K)Fe_xSe_2 compounds is studied from the viewpoint of doped Mott insulator. The Mott insulating phase is examined to be preferred in the parent compound at $x = 1.5$ due to the presence of Fe vacancies. Partial filling of vacancies at the Fe-sites introduces electron carriers and leads to electron doped superconductivity. By using a two-orbital Hubbard model in the strong coupling limit, we find that the s-wave pairing is more favorable at small Hund's coupling, and $d_{x^2-y^2}$ wave pairing is more favorable at large Hund's coupling.

Copper-oxide and iron based superconductors are two families with the highest transition temperatures. [1–5]. In copper oxides, the parent compounds are antiferromagnetic (AFM) Mott insulators. Superconductivity arises when charge carriers are introduced by chemical doping. In Fe-based materials, the parent compounds are bad metals with AFM long range order. Superconductivity arises when the AFM ordering is suppressed by chemical doping. A common feature for the superconductivity in the two families is the nearby AFM states, so that it is generally believed that the superconductivity is closely related to the antiferromagnetism in both families. The important difference between the insulating phase in cuprates and the metallic phase in Fe-based parent compounds have been thought to distinguish the two classes of high Tc superconductors. In the theoretical description, the electron interaction is strong in cuprates and weak or intermediate in Fe-based compounds. This has prevented the development for a unified physical picture for the two families of high Tc superconductivity. Most theories for Fe-based superconductivity are based on a weak coupling approach to consider magnetic fluctuations as a pairing mechanism. [6] In these theories, the parent compound has a spin density wave ground state with the gap opening at only part of the Fermi surface, so that it is a metal. In the strong coupling theories, one starts with the assumed insulating parent state [7–9] and the theories could only applied to study the magnetism but have difficulties to explain metallic feature of the parent state.

Very recently, it has been reported that FeSe-layer compounds (Tl,K)Fe_xSe_2 are AFM insulators at $1.3 < x < 1.7$ and become superconductors at $1.7 < x < 1.88$ with $T_c = 31$K and $T_c^{\rm onset} = 40$K [10]. Note that there was an early report that $K_{0.8}Fe_xSe_2$ is superconducting. [5] The parent compound of this new family of iron selenide may be considered to be $Tl_{1-y}K_yFe_{1.5}Se_2$, where FeSe layers share a similar structure to FeAs layers in iron arsenic compounds with As^{3-} being replaced by Se^{2-} ions and 1/4 of Fe sites being vacant. The partial substitution of K by Tl is to stabilize the chemical component and to prevent the oxidization. This raises an interesting possibility that Fe-based superconductivity is also a doped Mott insulator, similar to the cuprates.

In this paper, we propose that the insulating state of Tl(K)$Fe_{1.5}Se_2$ is a Mott insulator due to the Fe-vacancies, which enhance the electron correlation. The argument is substantiated by a model calculation involving the vacancies and the on-site Coulomb and Hund's coupling. We use a strong coupling theory of two band model to show that partial filling of the Fe-vacancies leads to s-wave superconductivity, which is compatible with the strong disorder in the system.

We start with the insulating compound Tl(K)$Fe_{1.5}Se_2$. The vacancies form a superlattice as suggested in early work and in the recent transmission electron microscopy on KFe_xSe_2 for $1.5 \leq x \leq 1.6$. [11, 12] The two possi-

ble super-lattice structures are illustrated in Fig. 1, which may be stabilized by the Coulomb repulsion of the Fe-ions. In this compound, we have all Fe^{2+} or configuration of Fe-3d^6. Local density approximation (LDA) calculations show a metallic ground state, so that the state is clearly not a band insulator. The vacancy ordering is a strong evidence that the insulating phase is not due to disorder effect or the Anderson localization. We argue that the insulating phase is also difficult to be explained due to a spin density wave ordering. The gap opened due to spin density wave ordering is usually at part of the Fermi surface of the normal state. A full gap at every Fermi point would require particle-hole symmetry in the electronic structure, which is not supported by either LDA calculations [13]or angle resolved photoemission spectroscopy(ARPES) data [14]. The insulating state requires a full gap opening on the Fermi surface, pointing out the strong electron correlation effect or the Mottness physics nature of the compound.

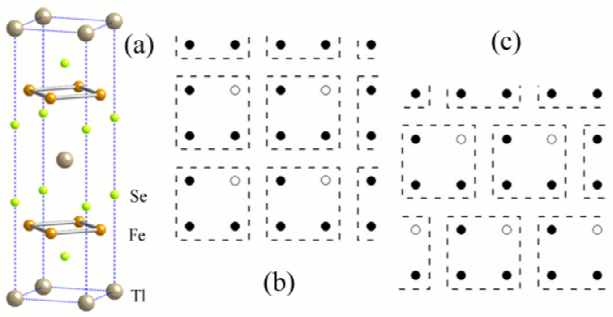

Fig. 1: (Color online) $TlFe_xSe_2$ with $ThCr_2Si_2$ type structure. (a) a unit cell without vacancy; (b) Fe square layer with 1/4 vacancy ordered in square; (c) Fe square layer with 1/4 vacancy ordered in parallelogram. The filled circles denote Fe atom while the empty circles are for vacancies. The squares by the dash lines denote the unit cells. Note that we ignore the up-down distribution of Se atoms which will result in doubly enlarged unit cells in parallelogram case.

Since the parent compounds of Fe-based superconductors in the absence of Fe-vacancies are metals, the insulating nature of Tl(K)Fe_xSe_2 is expected to be related to the Fe-site vacancies. In the presence of 1/4 Fe-vacancies, the number of bonds for each Fe-atom to connect with the nearest neighbor (NN) and the next nearest neighbor (NNN) Fe-atoms is reduced from 8 to 16/3, so that the kinetic energy of Fe-3d electron is substantially reduced. Note that the electron hopping integrals at NN and NNN sites are most important kinetic terms in a tight-binding description for the Fe-based materials. This enhances the on-site Coulomb repulsion relative to the kinetic energy, hence the electron correlation. In this scenario, Fe-based compounds are at the boundary of metal-insulator transition, and may be "tunable" by introducing superlattice vacancies. The superconductivity is induced by chemical doping, which introduces charge careers in addition to the variation of the Fe-vacancies. Below we shall use a model to examine the metal-insulator transition associated with the Fe-vacancies and the superconductivity in the doped cases.

A generic microscopic model to describe Fe-layer in the system can be written down in terms of five $3d$ Fe orbitals, which reads

$$H = H_0 + H_I. \tag{1}$$

H_0 is a tight-binding Hamiltonian given by

$$H_0 = -\sum_{i,\vec{\tau},\alpha\beta\sigma} t_{\vec{\tau}}^{\alpha\beta} c_{i+\vec{\tau},\alpha\sigma}^{\dagger} c_{i\beta\sigma}, \tag{2}$$

where $t_{\vec{\tau}}^{\alpha\beta}$ is the hopping integral between two sites i and $j = i+\vec{\tau}$ with indices $\alpha, \beta = 1, 2, \cdots, 5$ for five 3d orbitals. H_I describes the on-site Coulomb interaction,

$$\begin{aligned} H_I &= \sum_{i,\alpha} U \hat{n}_{i\alpha\uparrow}\hat{n}_{i\alpha\downarrow} + \sum_{i,\alpha<\beta} J(\hat{c}_{i\alpha\uparrow}^{\dagger}\hat{c}_{i\alpha\downarrow}^{\dagger}\hat{c}_{i\beta\downarrow}\hat{c}_{i\beta\uparrow} + h.c.) \\ &+ \sum_{i,\alpha<\beta,\sigma\sigma\prime} (U'\hat{n}_{i\alpha\sigma}\hat{n}_{i\beta\sigma\prime} + J\hat{c}_{i\alpha\sigma}^{\dagger}\hat{c}_{i\beta\sigma\prime}^{\dagger}\hat{c}_{i\alpha\sigma\prime}\hat{c}_{i\beta\sigma}) \end{aligned} \tag{3}$$

where $\hat{n}_{i\alpha\sigma} = \hat{c}_{i\alpha\sigma}^{\dagger}\hat{c}_{i\alpha\sigma}$, U and U' are the intra- and inter-orbital direct Coulomb repulsions, respectively. J is the Hund's coupling which satisfies $U = U' + 2J$ by symmetry.

From quantum chemistry point of view, both the valence of Fe ions and the buckling of Se ions are similar to those in iron arsenides, we argue that the low energy electronic states are mainly Fe-3d_{xz} and 3d_{yz} orbitals. Therefore, we may adopt a 2-orbital model to study the Mott insulator transition and the superconductivity at large U limit. Within this 2-orbital model, 3$d_{x^2-y^2}$ and 3d_{3z^2} orbitals are completely occupied and 3d_{xy} orbital is completely empty, so that Fe-3d^6 has two electrons, and Fe-3d^7 has three electrons or one hole in the subspace of 3d_{xz} and 3d_{yz} orbitals. The simplified 2-orbital model takes similar form of Eqs.(1,2,3), while $\vec{\tau}$ is for the NN and NNN bonds only and the orbital indices $\alpha, \beta = 1$ or 2 are for orbital d_{xz} and d_{yz} respectively. We further set $t_{\hat{x}}^{11} = t_{\hat{y}}^{22} = t_1$, $t_{\hat{y}}^{11} = t_{\hat{x}}^{22} = t_2$, $t_{\hat{x}\pm\hat{y}}^{\alpha\alpha} = t_3$, and $t_{\hat{x}\pm\hat{y}}^{12} = \pm t_4$ by lattice and orbital symmetry as in iron pnictides. Within the 2-orbital band model, there are two electron per Fe-ion in the parent compound Tl(K)$Fe_{1.5}Se_2$. We study metal to Mott insulator transition by using a slave spin technique [15]. The main results are shown in Fig.2. For a given J/U, one sees that the renormalized quasiparticle weight Z decreases as U/W increases and vanishes at $U = U_c$, with W the bandwidth of the system in the absence of Fe-vacancy. Our calculations show that the critical value U_c for the Mott transition is reduced in the presence of the vacancy, and the reduction becomes more profound due to the Hund's coupling J. The role of Hund's coupling to the reduction of U_c in multiple- orbital systems has been studied previously by using slave spin study on iron pnictides in the absence of Fe-vacancy [16].

Electron doping to the parent compound is realized by partial filling of the Fe-vacancies in the parent compound.

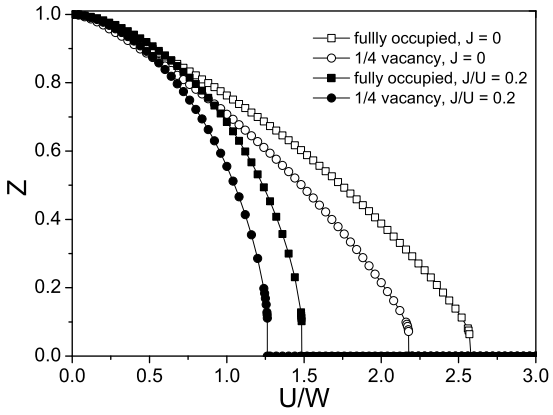

Fig. 2: Quasiparticle weight Z decreases with increasing U and fixing J/U. U_c is reduced when vacancy are presented, where the hopping integrals are chosen to be $t_1 = -t, t_2 = 1.3t, t_3 = t_4 = -0.85t$, and $W = 12t$ is chosen to be the bandwidth for fully occupied Fe lattice. Vacancies occupy 1/4 Fe sites and forms a square lattice as shown in Fig.1(b). Note that the results for parallelogram ordered vacancies as shown in Fig.1(c) is quite similar.

This results in possible superconductivity at low temperatures. Below we shall examine the pairing interaction of the 2-orbital Hubbard model from a viewpoint of the doped Mott insulator. In the superconducting phases, say, $1.7 < x < 1.88$, vacancy density becomes lower and a variety of microstructures may coexist. The average number of electrons per site in the Fe-layer is $4 - \frac{3}{x}$ at the composition Tl(K)Fe_xSe_2 as required by the charge balance. At $x > 1.5$, some of the lattice sites have three electrons (or one hole) within the two-orbital model considered here. These holes move in the lattice background of Fe-ions with two-hole per site. The effective interaction between two single hole on the neighboring sites (i,j) can be derived by using second order perturbation theory in the large (U, J) limit by considering the virtual hopping processes [9], similar to the super-exchange interaction derived in the single band Hubbard model. In terms of fermionic representation, this effective interaction H_2 can be written in Eq.(4) below. We note that the spin coupling term has been included in study of the Gossamer superconductivity within the single band Hubbard model [17].

$$H_2 = -\sum_{ij}\sum_{\alpha\beta\alpha'\beta'}\Big[A_{\alpha\beta}^{\beta'\alpha'}(ij)\hat{b}_{\alpha\beta}^{\dagger}(ij)\hat{b}^{\alpha'\beta'}(ij) + \sum_{S_z} B_{\alpha\beta}^{\beta'\alpha'}(ij)\hat{T}_{\alpha\beta}^{S_z\dagger}(ij)\hat{T}_{S_z}^{\alpha'\beta'}(ij)\Big] \quad (4)$$

where $S_z = -1, 0, 1$, and

$$A_{\alpha\beta}^{\beta'\alpha'}(ij) = [\frac{(-1)^{\beta+\beta'}}{U-J} + \frac{1}{U+J}]t_{ij}^{\alpha\beta}t_{ji}^{\beta'\alpha'} + \frac{t_{ij}^{\alpha\bar{\beta}}t_{ji}^{\bar{\beta}'\alpha'}}{U'+J}$$
$$B_{\alpha\beta}^{\beta'\alpha'}(ij) = \frac{(-1)^{\beta+\beta'}}{U'-J}t_{ij}^{\alpha\bar{\beta}}t_{ji}^{\bar{\beta}'\alpha'}, \quad (5)$$

where $\bar{\beta}$ indicates the orbital different from β, and the first and the second terms in H_2 are the pairing interaction in the spin singlet and spin triplet channel, respectively.

We now proceed to discuss the superconducting pairing symmetry. As discussed above, vacancies are distributed randomly at Fe layers in superconducting phase and behave similar as non-magnetic impurities. The spin singlet s-wave superconductivity is essentially unaffected by non-magnetic impurities due to Anderson's theorem [18], but is strongly affected by magnetic impurities [19]. On the other hand, a p-wave superconductor with spin triplet is very sensitive to both non-magnetic and magnetic impurities [19]. This explains why spin triplet p-wave superconducting state Sr_2RuO_4 requires clean sample and also suggests that the spin triplet pairing is unlikely in this material. So we will only consider the spin singlet pairing below.

Fang et al.'s experiment has suggested that there are several superconducting transitions in the material [10]. This result is consistent with the observed microstructures of the TEM $KFe_{1.8}Se_2$ [12] where both the domains with many ordered vacancies and the domains with very few randomly distributed vacancies are found. As Fe content increases, both the superconductivity and the total area of the domains with randomly distributed vacancies increases. As the first step, we approximate the disordered system with an average of $4 - 3/x$ electron per Fe-site on the Fe-layer. Note that the approximation has an exact limiting case of no vacancy at $x = 2$, which corresponds to 2.5 electrons per Fe ion.

By diagonalizing the mean field Hamiltonian of the two orbital model, one will have two bands [9], the upper and lower bands with energy $\epsilon_{\mathbf{k}\pm}$, respectively. Even in the case with a large electron concentration, both of the two bands will still across the Fermi energy and give two electron pockets around X and Y points and two hole pockets around Γ and M points. On the other hand, the ARPES has suggested the disappearance of the hole pockets [14]. This discrepancy may be due to the momentum dependent shift of the Fermi energy in comparing the ARPES and LDA results [20]. To resolve this discrepancy, here we shall take a phenomenological approach to assume that the lower bands are fully occupied and only the upper bands are considered. The electron carrier concentration is then $\delta = 2 - \frac{3}{x}$. In the following, we will consider the case with $\delta = 0.3$ which corresponds to $x \approx 1.76$.

In a random Fe-site vacancy approximation, the symmetry analysis for superconductivity studied previously for Fe-pnictides can be applied here, which suggests four possible pairing symmetries in the even-parity spin-singlet

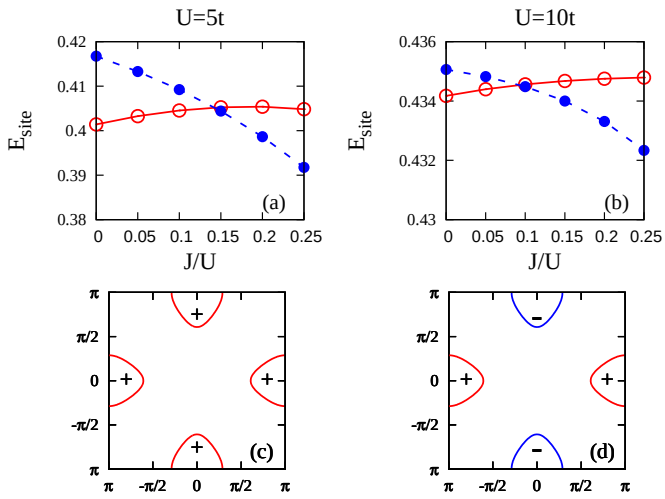

Fig. 3: (a) and (b), The energy of s-wave-like (red solid line) and d-wave-like (blue dashed line) pairing symmetry at $U = 5t$ and $U = 10t$, respectively. The electron doping is $\delta = 0.3$. (c) and (d), the schematic diagram of gap function of A_{1g} and B_{1g} pairing symmetry, respectively. The former one is like a s-wave pairing while the latter one is like a d-wave pairing. The sign in each pocket indicate the sign of the gap function. The gap function on the Fermi surfaces with same color has same sign.

case, i.e. A_{1g}, A_{2g}, B_{1g} and B_{2g} [21]. So we perform a mean field calculation similar to that in our previous work [9] to study the pairing symmetries in FeSe layer compounds. The main difference here is that we only consider the pairing between the electrons in the upper band because the lower band is fully occupied. Similar with the iron pnictide case, the pairing amplitude in A_{2g} and B_{2g} channel is very tiny and will not be discussed further. The energy of A_{1g} and B_{1g} pairing symmetries for various J/U with $U = 5t$ and $U = 10t$ are depicted in Fig. 3. We see that the A_{1g} pairing symmetry has lowest energy when J/U is small while the B_{1g} wins when J/U is large. This result is also consistent with the qualitative analysis based on the pair hopping terms [9]. One difference from the iron pnictide is that B_{1g} is easier to win in the FeSe layer compounds, which may be due to the lack of the pairing hopping between electron pocket and hole pocket, which favors A_{1g} symmetry.

By carefully checking the quasi-particle gap on the Fermi surface, we find that the gap on each electron pockets are nodeless and rather isotropic for both A_{1g} and B_{1g} pairing symmetries. But the gap function of A_{1g} symmetry have same sign on different electron pockets, while the one of B_{1g} symmetry have different sign on electron pockets around X and Y point, respectively as shown in Fig. 3(c) and (d). This indicates that A_{1g} symmetry is like s-wave while B_{1g} symmetry is d-wave. But this "d-wave" symmetry is nodeless in contrast with the conventional d-wave symmetry.

ARPES experiments show that the superconductor gap is nodeless and almost isotropic. [14] So that the "s-wave" pairing state appears consistent with ARPES. However, the "d-wave" like pairing state can not be ruled out since it is nodeless and the anisotropy is weak.

The random distribution of Fe vacancies will introduce non-magnetic disorder effect. Roughly speaking, the vacancies will not affect the "s-wave" pairing state drastically, but will suppress the superconductivity for other non-s-wave SC states, including the "d-wave" like state. However, the disorder effect in such superconducting systems is a subtle and interesting issue and we will leave detailed analysis for future study . We speculate that the non-magnetic impurities act as what they do in dirty two-band superconductors as studied by Ng using Ginzburg-Landau theory. [23] Non-magnetic impurities scatter an electron between X and Y pockets with scattering rate τ_t^{-1}, where τ_t is the mean lifetime an electron stays in one pocket. In the weak scattering regime $\tau_t^{-1} \ll$ the transition temperature T_c or the gap Δ, the superconductor behave as "d-wave" like, while in the strong scattering regime $\tau_t^{-1} \gg T_c, \Delta$ the superconductor behaves as "s-wave" like.

In summary, we studied the Mottness and superconductivity in (Tl,K)Fe_xSe_2. By using the slave spin method, we find that the superlattice vacancies in the parent compound of x=1.5 enhance the electron correlation and lead to transition to a Mott insulator. We predict a sizable gap due to the electron correlation in the parent compound ($x = 1.5$), which should be observable in optical measurement [24]. Treating Fe vacancies randomly distributed, we find that a spin-singlet superconductor is likely at such a doped Mott insulator at $1.7 < x < 1.88$. The s-wave pairing is more favorable at small Hund's coupling, and $d_{x^2-y^2}$ wave pairing is more favorable at large Hund's coupling. In our theory, the intra-pocket pairing is dominant, the superconductivity is not relying on the inter-pocket pairing between electron and hole pockets, consisting with the observed superconducting in only electron pocket systems. While our study is based on 2-orbital Hubbard model, the essential physics should remain qualitatively unchanged if more orbitals are included. It would be interesting to see the possibility that the insulating state of the parent compound of x=1.5 become superconducting under a high pressure, similar to that in layered organic superconductivity [17, 22]

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Note: Near the completion of this work, we learned a similar work by Yu et al. [25], where Mott transition at $x = 1.5$ compound is studied.

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